OST TECHNICAL PROGRESS REPORT

TEAM WORK PLAN--FY 2001 RESULTS

TITLE: Simulation and Modeling

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DESCRIPTION:

The Simulation and Modeling Team's activities focus on supplying insight for the design and operation of devices used by the power generation or chemical industries. Developing and using computational models provides the insight. Because a large variety of such devices exist and because each model represents a trade-off between accuracy and speed, a large variety of modeling approaches is used. The Team's activity is comprised of many distinct efforts all related to developing and using computational tools to help contractors and experimentalists further develop NETL's technologies. The activity includes:

1) Exploring the suitability of particle based methods, especially smoothed particle hydrodynamics (SPH).

2) Develop computational fluid dynamics (CFD) capabilities for heavily loaded gas/particle flows.

3) Develop and validate CFD models to predict filter vessel performance.

4) Use three-dimensional CFD to simulate combustor and combustion systems.

5) Development and testing of a Kalman filter on NETL's circulating fluidized bed (CFB).

6) Development of constitutive laws for flowing granular solids.

RESEARCH OBJECTIVES:

1) The SPH approach transforms complex partial differential equations (PDE) that represent a continuum field view into a corresponding set of ordinary differential equations (ODEs) which represent a pseudo-particle view. This is done via integral equations and smoothing. The research has two parts. The first result will be a working model that uses the SPH framework to calculate flows. The second result is the development of tools and methods that bridge the gap between engineering analysis, which uses lumped thermodynamic models, and an analysis that uses first-principles physical models. Successful completion of these two objectives will allow SPH methods to quickly calculate the distributed fluid flows in complex engineered systems so that the results may be graphically rendered in the form of virtual reality demonstrations.

2) In order to utilize the cluster computer architecture, we continue to improve and validate the NETL-developed CFD code, MFIX. Implementation of frictional flow capabilities within the MFIX code has allowed the description of a dense particle flow regime. Numerical improvements to MFIX have been made to enhance its accuracy and robustness.

3) The objective is to simulate the flow and thermal behavior in the particulate filter vessel at the PSDF in Wilsonville, Alabama in order to provide insight into the development of reliable techniques to remove particulate matter from high-temperature, high-pressure gas streams produced from coal combustion and/or gasification processes.

4) Model the influence of electric fields on flames for the development of a flame sensor and adapt a methodology for converting known frequency domain boundary impedance into a numerical boundary condition for nonlinear CFD codes.

5) Finish developing the Kalman filter to characterize the operating behavior of NETL's CFB using real data in real time.

6) Ongoing derivation and testing of stress tensor expressions for granular flows.

LONG TERM GOALS / RELATIONSHIP TO NETL s PRODUCT LINE(S):

1) The long-term goal of this work is to develop a breakthrough for quickly solving complex fluid flow problems and graphically rendering the results. Success will benefit the Vision 21 Product Line by being able to quickly visualize the affect of a modification to a plant.

2) Fluidized bed processes are now a standard unit operation in the power industry. They are utilized in coal (or biomass) gasification and combustion processes and in clean-up processes. Other operations, such as cyclone separation or hot-gas filtration, involve dense gas/particle flows. The numerical techniques and code structure used in MFIX is also immediately relevant to bubble-column technology.

The design of advanced (and existing) processes of energy conversion requires the prediction of the behavior of dense gas/solid flows. Operations such as fluidized bed, pneumatic transport, and hopper flow are used throughout the power industry and in related industries such as chemical, petrochemical and pharmaceutical. Within these industries, processes that involve gas/particle flow are much less reliable, due to design uncertainties. This results in drastically increased operational costs. CFD provides a science-based method for the design of these devices. Within these industries, CFD is now routinely used for the analysis of reactive, single-phase flows and even dilute gas/solid flows. However, CFD for heavily loaded gas/particle flows is a much more difficult challenge, requiring major numerical and theoretical modifications of the single-phase methods.

2) As part of the Clean Coal Technology Program at the U.S. Department of Energy, advanced pressurized fluidized bed combustors (PFBC) and integrated gasification combined cycle (IGCC) systems are being developed and tested. These highly-efficient coal-fired electricity generating systems require effective removal of particulate from the hot gases to protect the downstream gas turbine components from particulate fouling and erosion effects and to clean the gas to meet particulate emission requirements. The current hot-gas filtration technology is focused on the use of candle filters. They generally have a very high cleaning efficiency and deliver essentially particulate-free hot gases that meet turbine engineering requirements and regulatory standards for power-plant emissions. However, there are a number of unresolved problems with buildup of dust cake on the filters, occasional filter-ash bridging, and filter failure and breakage.

To design effective and reliable hot-gas cleaning filtration systems, a fundamental understanding of the particle transport and deposition processes in filter vessels is needed. Modeling of gas flow and particle transport and deposition is one important technique available in advancing our knowledge of the mechanism by which particle deposits begin and grow.

4) The prevention of the large-scale acoustic fluctuations associated with combustion instabilities is needed to prevent damage to the gas turbine engine. Modern gas turbine combustors must operate near the lean extinction limit to minimize the amount of pollutants formed. At this operating condition the combustor is particularly susceptible to combustion instabilities. Furthermore, the desired operating condition must be controlled within close tolerances of the design point, despite changes in the flow splits due to manufacturing tolerances, engine wear, and momentary changes in fuel delivery. These two projects attempt to address these concerns using numerical simulation. The numerical simulation is used to investigate physical phenomena and as a testbed to develop new strategies to address these problems.

5) CFBs are popular devices used to react a granular solid with a fluid because of high solids-fluid contacting. However, their operation is imperfectly understood, and the ability to operate a CFB optimally would greatly increase their efficiency. A Kalman filter has the potential for doing so. Kalman filters have been employed to optimally run electrical devices such as motors in which time is the only independent variable. We are developing Kalman filters for devices in the power generation and chemical process industries in which space is also an independent variable.

6) Much of NETL's technologies are involved with processing granular solids like coal or sawdust. Simulations of those technologies require mathematical expressions relating how those materials deform and flow in response to a stress and how heat is transferred. Constititutive law development and testing for different materials under different conditions are ongoing activities and are necessary to insure simulation validity.

SUMMARY ACCOMPLISHMENTS:

1) This is a new project that was proposed at the Computational Energy Sciences Merit Review held at NETL in October 2000. The project was favorably reviewed, and funding has been secured to start the project.

2) Fourth-order spatial discretization has allowed greater numerical accuracy. This is important in describing the hydrodynamic properties of beds, such as "bubble" properties and cluster formation. High-order accuracy is required for large eddy simulations.

3) Our paper describing the computer simulation of gas flow and thermal behavior based on the Reynolds stress transport turbulence model has been accepted for publication in the NETL Journal of Energy and Environmental Research. Previous modeling studies were limited to isothermal conditions. However, researchers at the PSDF in Wilsonville, Alabama have reported temperature variations in the hot-gas filter vessel. These experimental findings have prompted NETL researchers to improve earlier models to include heat transfer. In this paper we have predicted that the temperature distribution is non-uniform with somewhat higher temperatures in the upper part of the filter vessel. The simulated gas temperature distributions in the vessel qualitatively agree with the field observations in the filter vessel. Results reveal that the gas flow shows strong rotating flow regions inside the filter vessel. Dr. Guan from Southern Company at the PSDF stated, "It is very nice to see the temperature distribution inside the vessel that was not available in previous simulations". He further indicated that they would like to work with us on future simulation work.

4) A new activity, no results are yet available.

5) "A State Estimation of the Standpipe of a Circulating Fluidized Bed using an Extended Kalman Filter," Hoowang Shim, Parviz Famouri, William N. Sams and Edward J. Boyle, 16th International Fluidized Bed Conference, Reno, NV, 2000.

6) "The effect of Slip Boundary Condition on the Flow of Granular Materials: A Continuum Approach," M. Massoudi, and T. X. Phuoc, International Journal of Non-Linear Mechanics, Vol. 35, pp.745-761, 2000.

"On the Flow of a Fluid-Particle Mixture Between Two Rotating Cylinders, Using the Theory of Interacting Continua," M. Massoudi and G. Johnson, International Journal of Non-Linear Mechanics, 35, pp. 1045-1058, 2000.

"Vertical Flow of a Multiphase Mixture in a Channel," M. Massoudi and C. Lakshmana Rao, Mathematical Problems in Engineering, 6, pp. 505-526, 2001.

"On the Flow of Granular Materials with Variable Material Properties," M. Massoudi, International Journal of Non-Linear Mechanics, 36, pp. 25-37, 2001.

"A Continuum-Kinetic Theory Approach to the Rapid Flow of Granular Materials: The Effects of

Volume Fraction Gradient." Mehrdad Massoudi and Edward Boyle, International Journal of Non-Linear Mechanics, 36, pp. 637-648, 2001.

"On the Importance of Material Frame-Indifference and Lift Forces in Multiphase Flows," M. Massoudi, NETL Journal of Energy and Environmental Research, 1, pp. 63-90, 2001.

"Flowing Granular Material and the Maxwell-Boltzmann Velocity Distribution," E.J. Boyle, Recent Advances in the Mechanics of Structured Continua – 2000 AMD 244 and MD 92, pp. 139-146, 2000.

"Derivation of the Two-Granule Distribution Function for the Reference State Flow," E.J. Boyle, NETL Journal of Energy and Environmental Research, 1, p. 105, 2001.

RESULTS:

1) Not applicable.

2) Publications and presentations resulting from this work are:
"Simulation of the Hydrodynamic Behavior of a Bubbling Fluidized Bed" T. J. O'Brien and M. Syamlal, Fluidization X: Fluidization for Sustainable Development, Beijing, 2001.

"The Effect of Numerical Diffusion on Isolated Bubbles in a Gas-Solid Fluidized Bed," Chris Guenther and Madhava Syamlal, Powder Technology, 2001. The finite volume method is used in MFIX to discretize the system of PDEs. Central to this process is the approximation of convective fluxes at cell faces. There are a variety of interpolation schemes that can be used in this approximation. Inherent in these schemes is numerical diffusion and an understanding of the effect of numerical diffusion in gas-solids fluidized beds is extremely important. The investigation of this was finished in FY00 and the results summarized in this paper.

NETL's CFB was simulated several times in an ongoing effort to validate MFIX and understand CFB technology. The results obtained in FY00 showed a discrepancy between different spatial discretization schemes in MFIX. These results are not only surprising but are unique in that MFIX is not always under predicting the riser pressure drop, which is a common problem throughout the research community. With the availability of experimental data currently being generated at NETL using cork particles, one of the goals of this project for FY01 is to determine how such discrepancies in the riser pressure drop occur and demonstrate that MFIX can predict the correct riser pressure drop. These results are being summarized for publication at the Seventh International Conference on Circulating Fluidized Beds.

3) Publication:
"Non-Isothermal Simulation of Gas Flows in the Hot-Gas Filter at Wilsonville," Isaac K. Gamwo Goodarz Ahmadi, and John S. Halow , accepted for publication in the NETL Journal of Energy and Environmental Research.

4) This is new research, and there are no findings to report.

5) NETL funds have been augmented by winning an EPSCoR grant worth $150K/year for three years.

"A State Estimation of the Standpipe of a Circulating Fluidized Bed using an Extended Kalman Filter," Hoowang Shim, Parviz Famouri, William N. Sams and Edward J. Boyle. In this article, an Extended Kalman Filter (EKF) is used to estimate the distribution of solids in the standpipe of a circulating fluidized bed. The dynamic model of the flow within the standpipe is based on mass conservation and a modified Richardson-Zaki correlation. The integrated form of the Ergun equation is used to relate the pressure drop measurements to the amount and velocity of solids in the standpipe. The Kalman filter proceeds in the following steps,

1. Assign values for the diagonal and positive semi-definite matrices Q and R, which, respectively, represent the error in the measurements and dynamic models, and choose initial conditions for the void fractions along the length of the standpipe, $\underline{\hat{\varepsilon}}_k(+)$, and error covariance matrix $P_k(+)$.
2. The predicted state vector is determined from the nonlinear dynamic model, which describes how solids flow in the standpipe in response to an upset:
$$\underline{\hat{\varepsilon}}_k(-) = \underline{f}_{k-1}\left(\underline{\hat{\varepsilon}}_{k-1}(+)\right).$$
3. In order to apply a Kalman filter, the response of the dynamic model is represented as a first-order linear approximation. The Jacobian matrix of the non-linear dynamic model is calculated as
$$F_k\left(\underline{\hat{\varepsilon}}_k(+)\right) = \left.\frac{\partial \underline{f}_k\left(\underline{\varepsilon}\right)}{\partial \underline{\varepsilon}}\right|_{\underline{\varepsilon}=\underline{\hat{\varepsilon}}_k(+)}.$$
4. The *a priori* error covariance matrix is computed as
$$P_k(-) = F_{k-1}\left(\underline{\hat{\varepsilon}}_{k-1}(+)\right) P_{k-1}(+) F_{k-1}\left(\underline{\hat{\varepsilon}}_{k-1}(+)\right)^{T} + Q.$$
5. As with the dynamic model, the nonlinear measurement model is linearized. It's Jacobian matrix is
$$H_k\left(\underline{\hat{\varepsilon}}_k(-)\right) = \left.\frac{\partial \underline{h}_k\left(\underline{\varepsilon}\right)}{\partial \underline{\varepsilon}}\right|_{\underline{\varepsilon}=\underline{\hat{\varepsilon}}_k(-)}.$$
6. The Kalman gain matrix, K_k, which minimizes the *a posteriori* error covariance, is computed as
$$K_k = P_k(-) H_k\left(\underline{\hat{\varepsilon}}_k(-)\right)^{T} \left\{H_k\left(\underline{\hat{\varepsilon}}_k(-)\right) P_k(-) H_k\left(\underline{\hat{\varepsilon}}_k(-)\right)^{T} + R\right\}^{-1}.$$
7. The estimate of the pressure difference is determined from the measurement model, the integrated Ergun equation,
$$\underline{\hat{p}}_k = \underline{h}_k\left(\underline{\hat{\varepsilon}}_k(-)\right).$$
8. The corrected estimate of the state vector is determined as:
$$\underline{\hat{\varepsilon}}_k(+) = \underline{\hat{\varepsilon}}_k(-) + K_k\left\{\underline{p}_k - \underline{\hat{p}}_k\right\}.$$

This vector is the Kalman filter estimate of the void fraction profile in the CFB standpipe at time step k.

9. The *a posteriori* error covariance matrix is computed as

$$P_k(+) = \left\{ \mathrm{I}_N - K_k H_k \left(\hat{\underline{\varepsilon}}_k(-) \right) \right\} P_k(-),$$

where I_N is an $N \times N$ identity matrix.

Finally, the time step is incremented and we return to step 2.

6) Book:

Recent Advances in the Mechanics of Structured Continua, III (2000), edited by M. Massoudi and K. R. Rajagopal, New York:ASME Publications, New York.

Journal Papers:

1. Massoudi, M. and Rao, C. Lakshmana (2001). Vertical flow of a multiphase mixture in a channel. Mathematical Problems in Engineering, 6, pp. 505-526.

2. Massoudi, M. (2001). On the flow of granular materials with variable material properties. International Journal of Non-Linear Mechanics, 36, pp. 25-37.

3. Massoudi, M. and Mehrabadi, M. M. (2001). A continuum model for granular materials: Considering dilatancy, and the Mohr-Coulomb criterion. Acta Mechanica, 152, pp. 121-138.

4. Massoudi, M. and Boyle, E. J. (2001). A continuum-kinetic theory approach to the flow of granular materials: The effects of volume fraction gradient. International Journal of Non-Linear Mechanics, 36, pp. 637-648.

5. Massoudi, M. and Phuoc, T. X. (2001). Fully developed flow of a modified second grade fluid with temperature dependent viscosity. Acta Mechanica, 150, pp. 23-37.

6. Massoudi, M. and Rao, C. Lakshmana (2001). A non-linear constitutive relation for flowing granular materials. International Journal of Applied Mechanics and Engineering, 6, pp. 457-471.

7. Massoudi, M. (2001). Local non-similarity solutions for the flow of a non-Newtonian fluid over a wedge. International Journal of Non-Linear Mechanics, 36, pp. 961-976.

8. Massoudi, M. (2001). Averaged equations for developing flow of a fluid-solid mixture. International Journal of Applied Mechanics and Engineering, 6, pp. 1025-1049.

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